ABSTRACT

Structure factor bias in an electron density map for an unknown crystallographic structure is minimized by using information in a first electron density map to elicit expected structure factor information. Observed structure factor amplitudes are combined with a starting set of crystallographic phases to form a first set of structure factors. A first electron density map is then derived and features of the first electron density map are identified to obtain expected distributions of electron density. Crystallographic phase probability distributions are established for possible crystallographic phases of reflection *k,* and the process is repeated as *k* is indexed through all of the plurality of reflections. An updated electron density map is derived from the crystallographic phase probability distributions for each one of the reflections. The entire process is then iterated to obtain a final set of crystallographic phases with minimum bias from known electron density maps.